

10/664,544

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

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STRUCTURE FILE UPDATES: 18 JUL 2004 HIGHEST RN 712264-54-5
DICTIONARY FILE UPDATES: 18 JUL 2004 HIGHEST RN 712264-54-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

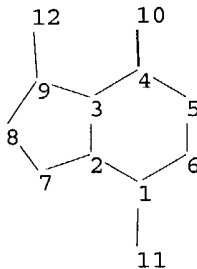
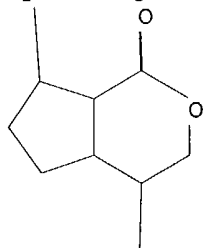
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=>

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chain nodes :

10 11 12

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

1-11 4-10 9-12

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9

exact/norm bonds :

4-10

exact bonds :

1-2 1-6 1-11 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9 9-12

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 15:25:59 FILE 'REGISTRY'

10/664,544

SAMPLE SCREEN SEARCH COMPLETED - 730 TO ITERATE

100.0% PROCESSED 730 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 12980 TO 16220
PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 15:26:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 14838 TO ITERATE

100.0% PROCESSED 14838 ITERATIONS 62 ANSWERS
SEARCH TIME: 00.00.01

L3 62 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 155.84 156.05

FILE 'CAPLUS' ENTERED AT 15:26:11 ON 19 JUL 2004
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FILE COVERS 1907 - 19 Jul 2004 VOL 141 ISS 4
FILE LAST UPDATED: 18 Jul 2004 (20040718/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 91 L3

=> s l4 and (process or make or made or sythesi? or produc? or method)
1955102 PROCESS
1297155 PROCESSES
2906486 PROCESS
(PROCESS OR PROCESSES)
192363 MAKE
147771 MAKES
330936 MAKE

10/664,544

(MAKE OR MAKES)
1102189 MADE
24 MADES
1102209 MADE
(MADE OR MADES)
33 SYTHESI?
3869767 PRODUC?
819279 PRODN
528 PRODNS
819459 PRODN
(PRODN OR PRODNS)
4270835 PRODUC?
(PRODUC? OR PRODN)
2638927 METHOD
1112225 METHODS
3438013 METHOD
(METHOD OR METHODS)
L5 32 L4 AND (PROCESS OR MAKE OR MADE OR SYTHESI? OR PRODUC? OR METHOD
)

=> s 15 and (hydrogenation or hydrogenate)
164124 HYDROGENATION
2057 HYDROGENATIONS
164328 HYDROGENATION
(HYDROGENATION OR HYDROGENATIONS)
1537 HYDROGENATE
423 HYDROGENATES
1924 HYDROGENATE
(HYDROGENATE OR HYDROGENATES)
L6 4 L5 AND (HYDROGENATION OR HYDROGENATE)

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1072192 HYDROGEN?
L7 5 L5 AND HYDROGEN?

=> dup rem 16 17
PROCESSING COMPLETED FOR L6
PROCESSING COMPLETED FOR L7
L8 5 DUP REM L6 L7 (4 DUPLICATES REMOVED)

=> d 18 ibib hitstr abs 1-5

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2003:818413 CAPLUS
DOCUMENT NUMBER: 139:307908
TITLE: **Production** of dihydronepetalactone by the
hydrogenation of nepetalactone in the presence
of supported Platinum-Group metal catalysts
INVENTOR(S): Manzer, Leo E.
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084946	A1	20031016	WO 2003-US10072	20030402

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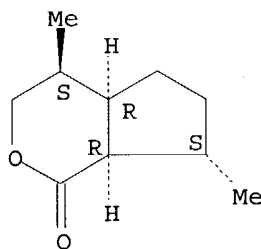
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003225290 A1 20031204 US 2003-405444 20030402
PRIORITY APPLN. INFO.: US 2002-369470P P 20020403
OTHER SOURCE(S): CASREACT 139:307908

IT 4581-72-0P, Dihydronepetalactone
RL: SPN (Synthetic preparation); PREP (Preparation)
(**production** of dihydronepetalactone by the **hydrogenation** of nepetalactone in the presence of supported Platinum-Group metal catalysts)

RN 4581-72-0 CAPLUS
CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4R,4aS,7R,7aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB A **process** for hydrogenating nepetalactone is described utilizing a metal catalyst (e.g., 5% Pd/C), that is optionally supported, to yield dihydronepetalactone in high yield and selectivity.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 1989:231890 CAPLUS

DOCUMENT NUMBER: 110:231890

TITLE: A new conversion **method** from (-)-limonene to nepetalactones

AUTHOR(S): Suemune, Hiroshi; Oda, Kozo; Saeki, Seitaro; Sakai, Kiyoshi

CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(1),

172-7

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:231890

IT 24190-26-9P 35337-14-5P

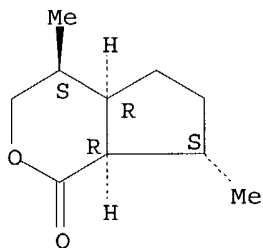
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled total synthesis of)

RN 24190-26-9 CAPLUS

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CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4S,4aR,7S,7aR) -
(9CI) (CA INDEX NAME)

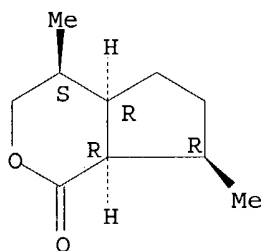
Absolute stereochemistry. Rotation (+).



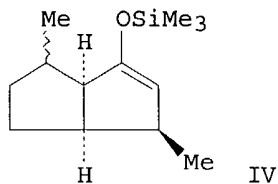
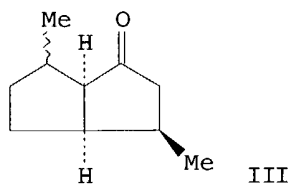
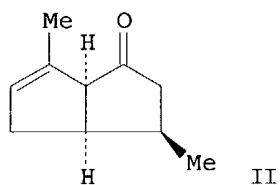
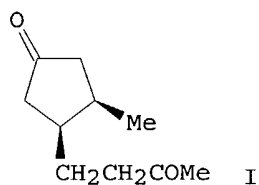
RN 35337-14-5 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4S,4aR,7R,7aR) -
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



GI



AB (-)-Limonene was converted to 4 nepetalactones in a stereocontrolled manner. The cis-3,4-disubstituted cyclopentanone I obtained from (-)-limonene via Rh(I)-catalyzed cyclization of the 4-pental, was converted to the bicyclo[3.3.0]octenone (II). After the stereoselective conversion of II into the diastereomeric isomers of ketones (III), a

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sequence of reactions involving the silyl enol ethers (IV), ozonolysis, and subsequent lactonization afforded the target mols.

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 1987:84374 CAPLUS

DOCUMENT NUMBER: 106:84374

TITLE: Claisen-rearrangement-mediated ring contraction of macrocyclic lactones. A new approach to carbocycles and heterocycles

AUTHOR(S): Funk, Raymond L.; Abelman, Matthew M.; Munger, John D., Jr.

CORPORATE SOURCE: Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA

SOURCE: Tetrahedron (1986), 42(11), 2831-46

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:84374

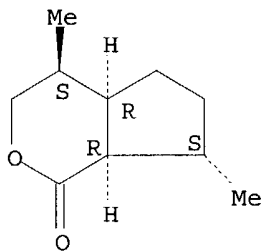
IT 4581-72-0P 17672-96-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 4581-72-0 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-,
(4R,4aS,7R,7aS)-rel- (9CI) (CA INDEX NAME)

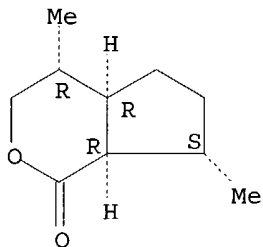
Relative stereochemistry.



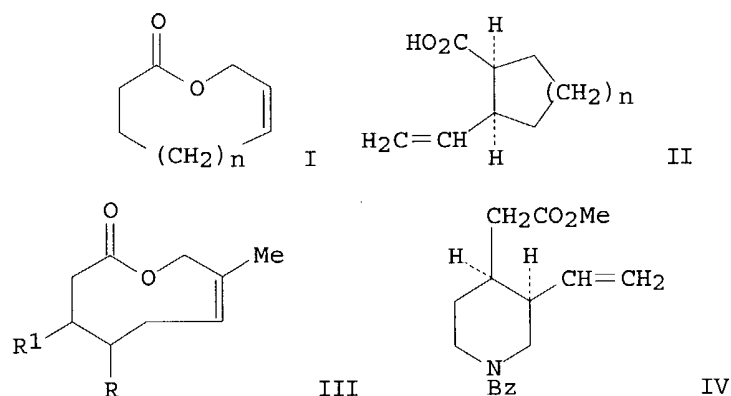
RN 17672-96-7 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-,
(4R,4aR,7S,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



AB Macrocyclic ketene acetals derived from lactones I ($n = 1, 2, 3, 4, 7$) undergo Claisen rearrangement smoothly and constitute a viable and general approach to hetero- or carbocyclic ring systems II. This novel ring contraction **process** is subject to high internal asym. induction, as well as relative asym. induction in the rearrangements of ketene acetals derived from lactones III ($R, R1 = H, Me$). N-Benzoylmerquinene Me ester IV was prepared to demonstrate the potential of this methodol. in heterocycle synthesis.

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 1981:117767 CAPLUS

DOCUMENT NUMBER: 94:117767

TITLE: New monoterpene lactones of the iridane type from Actinidia polygama Miq

AUTHOR(S): Sakai, Tsutomu; Nakajima, Kimiko; Sakan, Takeo

CORPORATE SOURCE: Suntory Inst. Bioorg. Res., Osaka, 618, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1980), 53(12), 3683-6

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 35337-15-6

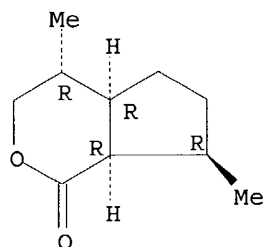
RL: FORM (Formation, nonpreparative)

(formation of, by catalytic **hydrogenation** of isoneonepetalactone)

RN 35337-15-6 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, [4R-(4 α ,4 α ,7 β ,7 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 76831-46-4 76831-47-5

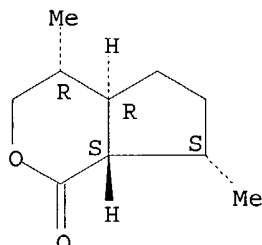
10/664,544

RL: BIOL (Biological study)
(from Actinidia polygama)

RN 76831-46-4 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4R,4aR,7S,7aS)-
(9CI) (CA INDEX NAME)

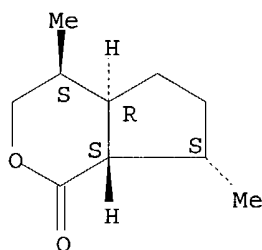
Absolute stereochemistry. Rotation (+).



RN 76831-47-5 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-,
[4S-(4 α ,4 β ,7 β ,7 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB Eight new iridoid monoterpene lactones (dihydroepinepetalactone, isodihydroepinepetalactone, isoepiiridomyrmecin, isoneonepetalactone, dehydroiridomyrmecin, isodehydroiridomyrmecin, actinidialactone, and isoactinidialactone), along with 5 previously isolated lactones (neonepetalactone, dihydronepetalactone, isodihydronepetalactone, iridomyrmecin, and isoiridomyrmecin), were isolated from the volatile oil of fresh fruits of the cat- and lacewing-attracting plant *A. polygama*. Also isolated from this oil was nepetalactone.

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1955:64532 CAPLUS

DOCUMENT NUMBER: 49:64532

ORIGINAL REFERENCE NO.: 49:12314a-h

TITLE: The degradation of nepetalactone

AUTHOR(S): Meinwald, Jerrold

CORPORATE SOURCE: Cornell Univ., Ithaca, NY

SOURCE: Journal of the American Chemical Society (1954), 76,
4571-3

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

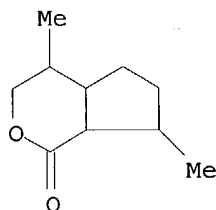
LANGUAGE: Unavailable

IT 21950-33-4, Cyclopentanecarboxylic acid, 2-(2-hydroxy-1-methylethyl)-5-methyl-, δ -lactone
(preparation of)

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RN 21950-33-4 CAPLUS

CN Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl- (8CI, 9CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB Nepetalactone was shown to possess structure I. Oil of catnip distilled by the method of McElvain, et al. (C.A. 36, 5800.2), yielded I, b13 129-30°, λ_{maximum} 5.67, 5.93 μ . Freshly distilled I (16.6 g.) in 50 cc. glacial AcOH **hydrogenated** several hrs. over 1.0 g. PtO₂, the mixture filtered, most of the AcOH distilled off in vacuo, the residue washed 3 times with H₂O and dissolved in Et₂O, the solution extracted with aqueous Na₂CO₃, the alkaline extract acidified with dilute HCl and extracted with

Et₂O, the extract washed, dried, and evaporated, and the residue distilled gave 11.6

g. 2-methyl-5-isopropylcyclopentanecarboxylic acid (II), b0.35 85°, n_{20D} 1.4568; the Et₂O layer (after extraction with the aqueous Na₂CO₃)

evaporated, and

the residue (4.2 g.) distilled gave dihydro derivative of I, b0.30 77-9°, λ_{maximum} 5.79 μ . II (6 g.) in 20 cc. dry Et₂O added with stirring to 5 g. LiAlH₄ suspended in 100 cc. dry Et₂O, the mixture stirred 5 hrs. at room temperature and decomposed with saturated aqueous Na₂SO₄, the aqueous

layer extracted twice

with Et₂O, and the combined Et₂O layer and extract dried and evaporated gave

5.3

g. 2-methyl-5-isopropylcyclopentylcarbinol (III), b0.70 60°, n_{20D} 1.4621, λ_{maximum} 3.0 μ . III (15.7 g.), 12.4 g. Ac₂O, and 9.6 g.

dry pyridine let stand overnight at room temperature, the mixture poured into

ice

water and extracted with Et₂O, and the extract washed with dilute HCl and H₂O yielded 17.9 g. acetate (IV) of III, b0.40 53°, n_{20D} 1.4467, λ_{maximum} 5.76 μ . Carborundum chips in a glass column heated to 500° and swept with N₂, 5.7 g. IV in 10 cc. pentane dropped through the column at a rate of 20 drops/min., the pyrolysis **product** collected in a Dry Ice trap, the collected yellow liquid having the odor of AcOH washed with base, the pentane distilled off, and the residue (4.2 g.) examined by infrared spectroscopy showed mainly unreacted IV with small

amts. of an olefin, λ_{maximum} 3.28, 6.07, 11.40 μ . IV (17.9 g.)

pyrolyzed similarly at 510° but without a diluent and the pyrolyzate worked up in the same manner gave 11 g. material shown to be IV mixed with an olefin; this mixture again pyrolyzed at 530°, and the resulting 7 g. pyrolyzate distilled gave 3 g. 2-methyl-5-

isopropylcyclopentylidenemethane (V), pale yellow oil, b150 84-90°, λ_{maximum} 3.28, 6.07, 11.40 μ , decolorized Br in CCl₄ and aqueous KMnO₄.

Crude V (2.8 g.) treated at -78° with excess ozone, the mixture poured into 8 g. Zn dust suspended in 25 cc. glacial AcOH, the mixture stirred 4 hrs. at room temperature, refluxed 1 hr., and distilled into 4.3 g. dimedon, 30 cc. 75% EtOH, and a few drops piperidine, and the mixture

concentrated

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to 20 cc. gave 1.25 g. dimedon derivative of CH₂O, m. 189-90°; the AcOH solution poured into H₂O and extracted with Et₂O gave 2.5 g. crude ketone, mobile yellow liquid, which distilled gave 1 g. 2-methyl-5-isopropylcyclopentanone (VI), b₇₄₀ 181-6°, λ_{maximum} 5.78 μ; 2,4-dinitrophenylhydrazone (VII), m. 169-71.5°. The infrared spectra of synthetic and natural VII and semicarbazone of VI are recorded.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

44.94

200.99

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.68

-3.68

STN INTERNATIONAL LOGOFF AT 15:30:01 ON 19 JUL 2004